

Chemistry 3370B: Organic and Inorganic Structure Elucidation 2022–23 Course Outline

Instructor: Prof. James Wisner

Office: Chemistry Building 215

Office Hours: By appointment; e-mail for an appointment. Students must use their Western (@uwo.ca) email addresses when contacting Prof. Wisner.

E-mail: jwisner@uwo.ca

Lectures and Tutorials

Section	Day	Time	Room
001	Tue	11:30 am – 12:20 pm	TC-204
	Thu	10:30 am – 12:20 pm	TC-204

The class notes will be posted to OWL at least 24 hours prior to the lectures.

Prerequisites

Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you will be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

Prerequisites for Chem 3370B: Either Chemistry 2273A and 2283G or Chemistry 2213A/B, either Chemistry 2271A and 2281G or Chemistry 2211A/B.

Course Description

Calendar description: Structure determination using common spectroscopic methods including vibrational and nuclear magnetic resonance spectroscopy as well as mass spectrometry and x-ray crystallography.

Course Topics

Class Topic
Administration, Introduction to Spectroscopy
Chapter 1: Molecular Formulas
Chapter 3: Mass Spectrometry <ul style="list-style-type: none">instrumentation; molecular weight determination; exact mass; isotopic clusters
Chapter 2: Infrared Spectroscopy <ul style="list-style-type: none">brief review of theory and important functional group frequencies and trends; interpretation of spectra
Chapters 5-9: NMR Spectroscopy <ul style="list-style-type: none">properties of magnetic nuclei and basic instrumentation; essential features of ^1H nmr spectra chemical shifts; ^{13}C and other heteronuclei nmr spectra; spin-spin couplings, magnitude of J; analysis of first order spectra, complex multiplets; chemical and magnetic equivalence and second order effects; OH/NH and dynamic processes; correlation spectroscopy
X-ray Crystallography <ul style="list-style-type: none">lattices, diffraction, understanding the data

Course Materials

Introduction to Spectroscopy, 5th Edition, Pavia/Lampman/Kriz/Vyvyan The text will be used extensively. It is a source of numerous problems to integrate the theory behind the spectroscopic techniques and practical experience. Note the useful appendices at the back of the book listing important spectral parameters. Also note questions with an asterisk (*) have answers provided at the back of the text.

Students should check OWL (<http://owl.uwo.ca>) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. Students are responsible for checking OWL on a regular basis. All course material will be posted to OWL: <http://owl.uwo.ca>.

If students need assistance, they can seek support on the OWL Help page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

There are many spectroscopy websites, and these are particularly useful:

General Spec: www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/spectro.htm#contnt

Reich's NMR site: www.chem.wisc.edu/areas/reich/chem605/index.htm

Notre Dame spectral problems: www.nd.edu/~smithgrp/structure/workbook.html

Learning Outcomes

The course also has an emphasis on the development of skills such critical-thinking, analysis, and qualitative reasoning; these professional skills are essential to success in not just chemistry but also in other courses and many occupations.

Course-Specific Outcomes

- Recognize the importance of spectroscopy in underpinning chemistry and the physical sciences.
 - Think critically about, explain, integrate, and apply spectroscopic principles and theories.
 - Recognize the diagnostic features of a variety of spectroscopic techniques.
 - Elucidate the structure of a compound using a variety of spectroscopic techniques.
 - Identify advantages and shortcomings in spectroscopic techniques.
-

Course Evaluation

The overall course grade will be calculated as listed below:

Component	Notes	Value
Problem Sets	6 at 5% each (Due dates: Feb 9, Feb 16, Mar 2, Mar 9, Mar 23, Mar 30 2022)	30
Midterm test	In-person, Saturday, March 11, 2022 at 12 pm – 2 pm, Location: TBA	30
Final Exam	In-person, Cumulative; 3 hours; Scheduled by the Registrar in the April Exam Period	40

Conditions required to pass the course: There are 6 problem sets in this course, each of these is a required component and their completion is a necessary element to help a student achieve the learning outcomes for this course. You must submit 4/6 problem sets to pass this course. In the event of accommodations reducing the number of assessments completed successfully below this minimum you will be required to complete the items missed the next time the course is offered. The evaluation weight from missed problem sets etc will be added to the remaining problem sets. There are no makeup problem sets.

The midterm test is a required component of the course and its completion is a necessary element to help a student achieve the learning outcomes for this course. If the midterm test is missed because of an approved accommodation, the evaluation weight from the missed midterm test will be added to the final exam. There is no makeup midterm exam.

Students who fail to meet any of these requirements without academic accommodation for the missed work will receive a course grade of not greater than 40%, even if the calculated grade is higher. A student who is unable to submit the required minimum number of assignments for medical or compassionate reasons, and who wishes to complete the missed work, will need to apply for Incomplete Standing (a grade of INC) by submitting a written request to the Dean of the Faculty of Registration. If

Incomplete Standing is granted, the student will be able to complete the missed items the next time the course is offered. A student who is unable to write the Final Exam must apply for permission to write a Special Final Examination (SPC Exam).

Policies

Student absences and missed work. Students who are unable to meet their academic responsibilities due to medical or compassionate reasons may submit a request for academic consideration. For each missed piece of work (regardless of its weight) you must apply for such consideration by providing valid medical or supporting documentation to the Academic Counselling Office of your Faculty of Registration. Note that all accommodations for missed work, regardless of who grants them, are subject to the Conditions required to pass the course.

Accommodation for students with disabilities. Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. In cases where a student misses a piece of work for reasons related to the disability on file with Accessible Education, the student should request accommodation by contacting Accessible Education instead of the Academic Counselling Office.

Missed assignments. There are no make-up assignments. If you miss an assignment and are granted accommodation, the weight of the missed assignment will be transferred to those that remain.

Missed midterm test. If you miss the midterm test and are granted accommodation, the weight of the midterm will be transferred to the Final Exam.

Missed Final Exam. If you miss the Final Exam, contact the Academic Counselling office of your Faculty of Registration as soon as possible. They will assess your eligibility to write the Special Examination. You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (e.g., more than 2 exams in 23-hour period, more than 3 exams in a 47-hour period).

Late assignments. All assignments must be submitted by 6:00 pm on the due date. A late penalty of 10% of the total grade for a problem set/day to a maximum of 3 days will be assessed for submissions before 6pm on subsequent dates. Students with applicable accommodations recommended by Accessible Education can request a longer one-time deadline extension. To preserve the integrity of evaluation, this extension cannot exceed 7 days after the regular due date because graded assignments and lab reports will normally be returned by that time. Students with disability accommodations who ask for a longer extension will be excused instead, subject to the Conditions required to pass the course.

Use of electronic devices. Only basic scientific calculators are permitted on all tests and exams. All other electronic devices (cell phones, laptops, tablets, cameras, etc.) are prohibited.

Scholastic offences. The University will take all appropriate measures to promote academic integrity and deal appropriately with scholastic offences. For definitions of what constitutes a scholastic offence, see http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf

Support Services. Detailed information on academic considerations for absences, religious accommodation, exam conflicts, appeals, and other academic matters may be found on the Science & Basic Medical Sciences Academic Counselling webpage: <https://www.uwo.ca/sci/counselling>. Students who are in emotional/mental distress should refer to Mental Health@Western (<https://uwo.ca/health>) for help.